Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:57 PM UTC

PDB ID	:	1INL / pdb_00001inl
Title	:	Crystal Structure of Spermidine Synthase from Thermotoga Maritima
Authors	:	Korolev, S.; Skarina, T.; Ikeguchi, Y.; Pegg, A.E.; Joachimiak, A.; Edwards, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2001-05-14
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

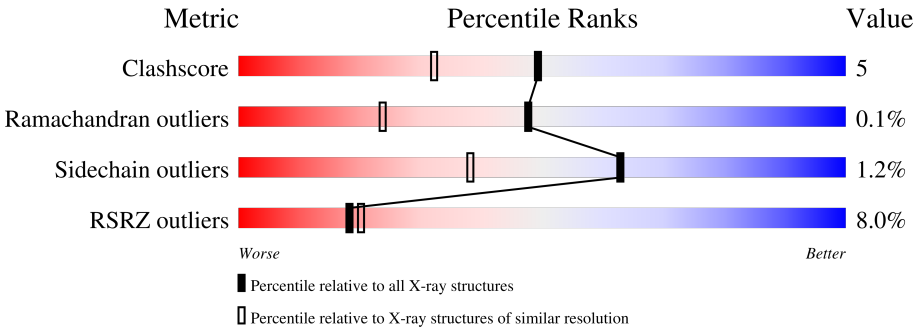
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	6% 90% 6% • •
1	B	296	7% 85% 10% • •
1	C	296	4% 89% 9% • •
1	D	296	13% 82% 12% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10234 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2326	1512	374	429	11			
1	B	291	Total	C	N	O	S	0	0	0
			2368	1537	382	438	11			
1	C	293	Total	C	N	O	S	0	0	0
			2382	1544	385	441	12			
1	D	282	Total	C	N	O	S	0	0	0
			2291	1487	370	422	12			

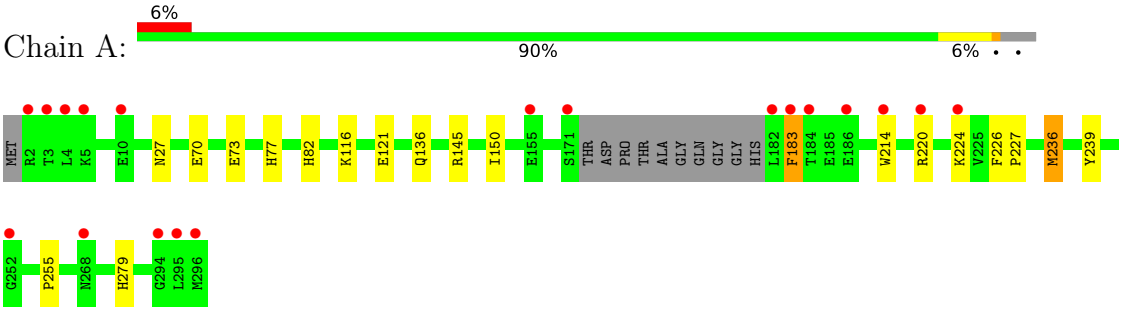
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	213	Total	O	0	0
			213	213		
2	B	244	Total	O	0	0
			244	244		
2	C	238	Total	O	0	0
			238	238		
2	D	172	Total	O	0	0
			172	172		

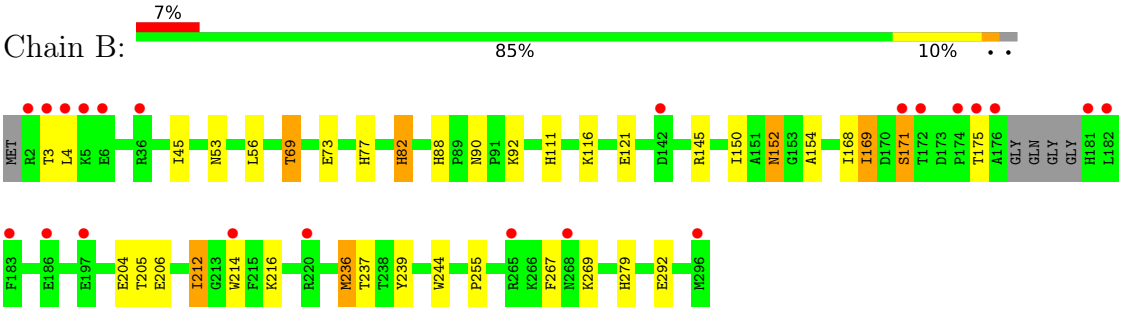
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

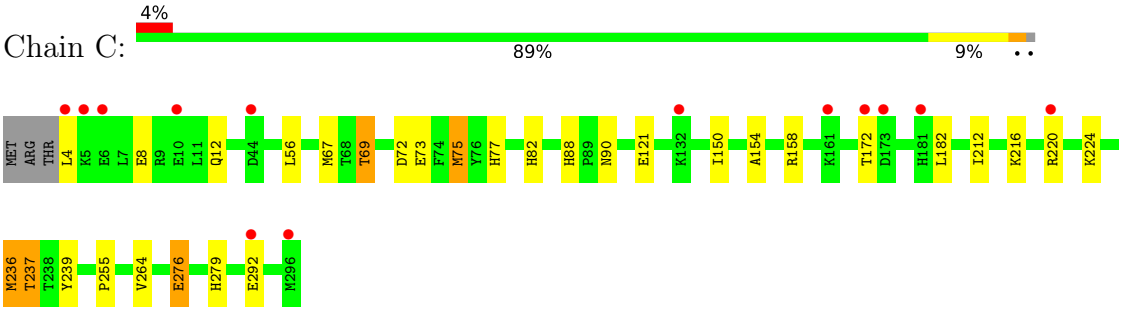
• Molecule 1: Spermidine synthase



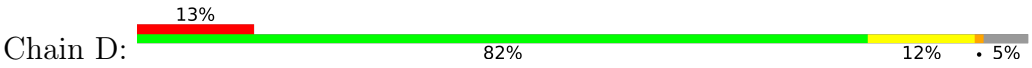
• Molecule 1: Spermidine synthase

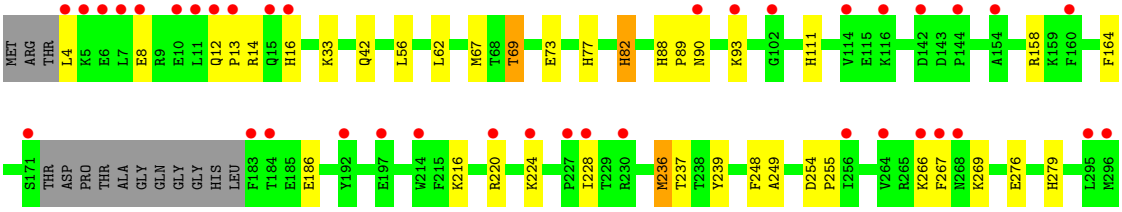


• Molecule 1: Spermidine synthase



• Molecule 1: Spermidine synthase




MET
ARG
THR
L4
K5
E6
L7
E8
R9
E10
L11
Q12
P13
R14
Q15
H16
K33
Q42
L56
L62
M67
T68
T69
E73
H77
H82
H88
P89
N90
K93
G102
H111
V114
E115
K116
D142
D143
P144
A154
R158
K159
F160
F164
S171
THR
ASP
PRO
THR
ALA
GLY
GLN
GLY
GLY
HIS
LEU
F183
T184
E185
E186
Y192
E197
W214
F215
K216
R220
K224
P227
I228
T229
R230
M236
T237
T238
Y239
F248
A249
D254
P255
I256
V264
R265
K266
F267
N268
K269
E276
H279
L296
M296

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.44Å 197.81Å 51.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 1.50 48.10 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.10-1.50) 95.3 (48.10-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.199 , 0.213 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10234	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/2385	0.83	1/3220 (0.0%)
1	B	0.35	0/2429	0.84	4/3282 (0.1%)
1	C	0.38	2/2444 (0.1%)	0.84	2/3301 (0.1%)
1	D	0.33	0/2349	0.85	5/3172 (0.2%)
All	All	0.35	2/9607 (0.0%)	0.84	12/12975 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	MET	SD-CE	-6.15	1.64	1.79
1	C	75	MET	SD-CE	-5.31	1.66	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	237	THR	N-CA-C	7.13	121.42	112.87
1	D	237	THR	N-CA-C	7.09	121.56	112.34
1	B	237	THR	N-CA-C	6.95	121.20	112.87
1	B	171	SER	N-CA-C	6.67	121.48	112.88
1	A	82	HIS	N-CA-C	6.39	119.24	111.82
1	D	82	HIS	N-CA-C	6.30	119.13	111.82
1	C	82	HIS	N-CA-C	6.22	119.03	111.82
1	B	82	HIS	N-CA-C	5.97	118.75	111.82
1	D	254	ASP	CA-C-N	5.25	125.56	119.47
1	D	254	ASP	C-N-CA	5.25	125.56	119.47
1	B	45	ILE	N-CA-C	5.24	116.15	111.90
1	D	276	GLU	N-CA-C	5.17	116.91	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2326	0	2274	13	0
1	B	2368	0	2306	31	0
1	C	2382	0	2327	33	0
1	D	2291	0	2227	26	0
2	A	213	0	0	1	0
2	B	244	0	0	2	0
2	C	238	0	0	2	0
2	D	172	0	0	0	0
All	All	10234	0	9134	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASP:HB2	1:C:75:MET:HE2	1.38	1.05
1:C:75:MET:HE1	1:C:237:THR:H	1.27	0.99
1:C:75:MET:HE3	1:C:236:MET:HE2	1.57	0.86
1:B:53:ASN:HD22	1:B:56:LEU:H	1.22	0.84
1:D:158:ARG:HH22	1:D:186:GLU:HG2	1.43	0.81
1:A:27:ASN:HD22	1:D:33:LYS:HD2	1.47	0.79
1:C:212:ILE:HD11	1:C:292:GLU:HG2	1.66	0.76
1:C:216:LYS:HD2	1:C:292:GLU:HG3	1.66	0.75
1:C:172:THR:HG21	1:C:182:LEU:HD12	1.70	0.73
1:B:88:HIS:HD2	1:B:90:ASN:H	1.41	0.67
1:D:248:PHE:CD2	1:D:255:PRO:HG3	2.29	0.66
1:D:158:ARG:NH2	1:D:186:GLU:HG2	2.10	0.66
1:B:169:ILE:HD12	1:B:169:ILE:N	2.13	0.64
1:B:88:HIS:CD2	1:B:90:ASN:H	2.15	0.63
1:C:88:HIS:HD2	1:C:90:ASN:H	1.46	0.61
1:C:88:HIS:CD2	1:C:90:ASN:H	2.18	0.61
1:C:75:MET:HE1	1:C:237:THR:N	2.09	0.61
1:B:73:GLU:OE1	1:B:77:HIS:HD2	1.84	0.60
1:B:82:HIS:ND1	1:B:111:HIS:HE1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:O	1:A:224:LYS:HD3	2.02	0.60
1:C:236:MET:HG3	1:C:239:TYR:CD2	2.37	0.60
1:A:73:GLU:OE1	1:A:77:HIS:HD2	1.85	0.59
1:C:73:GLU:OE1	1:C:77:HIS:HD2	1.86	0.58
1:D:73:GLU:OE1	1:D:77:HIS:HD2	1.87	0.57
1:A:183:PHE:HB3	1:A:214:TRP:CH2	2.40	0.57
1:C:172:THR:HG21	1:C:182:LEU:CD1	2.34	0.56
1:D:62:LEU:HB2	1:D:67:MET:HE3	1.88	0.55
1:D:220:ARG:O	1:D:224:LYS:HG2	2.07	0.55
1:D:93:LYS:HG3	1:D:164:PHE:CD1	2.43	0.54
1:A:236:MET:HG3	1:A:239:TYR:CD2	2.44	0.53
1:D:82:HIS:ND1	1:D:111:HIS:HE1	2.07	0.53
1:B:88:HIS:HE1	2:B:336:HOH:O	1.92	0.53
1:D:216:LYS:O	1:D:220:ARG:HG2	2.09	0.52
1:C:56:LEU:HB3	1:C:69:THR:HG23	1.90	0.52
1:B:3:THR:HG22	1:B:4:LEU:N	2.25	0.52
1:C:172:THR:CG2	1:C:182:LEU:HD12	2.40	0.52
1:A:27:ASN:ND2	1:D:33:LYS:HD2	2.23	0.52
1:D:236:MET:HG3	1:D:239:TYR:CD2	2.44	0.52
1:B:236:MET:HG3	1:B:239:TYR:CD2	2.46	0.51
1:B:3:THR:HG22	1:B:4:LEU:H	1.76	0.50
1:C:220:ARG:HG2	1:C:224:LYS:NZ	2.27	0.50
1:D:56:LEU:HB3	1:D:69:THR:HG23	1.94	0.50
1:B:152:ASN:ND2	1:B:154:ALA:H	2.10	0.50
1:B:77:HIS:HE1	2:B:322:HOH:O	1.95	0.49
1:B:90:ASN:ND2	1:B:92:LYS:HE3	2.28	0.49
1:B:56:LEU:HB3	1:B:69:THR:HG23	1.95	0.49
1:C:75:MET:CE	1:C:236:MET:HE2	2.38	0.48
1:C:77:HIS:HE1	2:C:316:HOH:O	1.95	0.48
1:B:255:PRO:O	1:B:279:HIS:HE1	1.96	0.48
1:A:255:PRO:O	1:A:279:HIS:HE1	1.98	0.47
1:C:255:PRO:O	1:C:279:HIS:HE1	1.97	0.47
1:B:168:ILE:C	1:B:169:ILE:HD12	2.40	0.47
1:D:266:LYS:HB2	1:D:266:LYS:NZ	2.30	0.47
1:B:169:ILE:N	1:B:169:ILE:CD1	2.77	0.47
1:C:12:GLN:H	1:D:42:GLN:HE21	1.62	0.46
1:A:70:GLU:HG3	1:A:136:GLN:NE2	2.31	0.46
1:D:255:PRO:O	1:D:279:HIS:HE1	1.99	0.46
1:B:152:ASN:HD21	1:B:154:ALA:HB3	1.82	0.45
1:C:212:ILE:CD1	1:C:292:GLU:HG2	2.43	0.45
1:C:264:VAL:HB	1:C:276:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:NZ	1:B:216:LYS:HB3	2.32	0.45
1:C:216:LYS:HD2	1:C:292:GLU:CG	2.40	0.45
1:C:220:ARG:HG2	1:C:224:LYS:HZ1	1.81	0.45
1:D:4:LEU:O	1:D:8:GLU:HG3	2.17	0.45
1:A:77:HIS:HE1	2:A:320:HOH:O	1.99	0.44
1:B:212:ILE:HD11	1:B:216:LYS:HD2	1.99	0.44
1:C:154:ALA:O	1:C:158:ARG:HG3	2.17	0.44
1:C:4:LEU:O	1:C:8:GLU:HG3	2.17	0.44
1:D:14:ARG:HB2	1:D:16:HIS:ND1	2.33	0.44
1:C:216:LYS:CD	1:C:292:GLU:HG3	2.43	0.43
1:D:248:PHE:CE2	1:D:255:PRO:HG3	2.53	0.43
1:C:121:GLU:O	1:C:150:ILE:HA	2.18	0.43
1:C:172:THR:CB	1:C:182:LEU:HD12	2.49	0.43
1:A:116:LYS:HD3	1:A:145:ARG:O	2.17	0.43
1:B:171:SER:HB3	1:B:204:GLU:CD	2.43	0.43
1:C:236:MET:HE2	1:C:236:MET:HA	2.01	0.43
1:C:75:MET:HE1	1:C:237:THR:OG1	2.19	0.42
1:B:171:SER:HB3	1:B:204:GLU:HG2	2.01	0.42
1:D:267:PHE:CE2	1:D:269:LYS:HB2	2.54	0.42
1:D:88:HIS:HD2	1:D:90:ASN:H	1.68	0.42
1:B:267:PHE:CE2	1:B:269:LYS:HB2	2.55	0.42
1:A:121:GLU:O	1:A:150:ILE:HA	2.19	0.42
1:B:205:THR:HA	1:B:214:TRP:HZ3	1.85	0.41
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.90	0.41
1:D:12:GLN:HA	1:D:13:PRO:HD3	1.81	0.41
1:B:116:LYS:HD3	1:B:145:ARG:O	2.20	0.41
1:B:121:GLU:O	1:B:150:ILE:HA	2.20	0.41
1:B:152:ASN:HD22	1:B:154:ALA:N	2.19	0.41
1:B:206:GLU:HA	1:B:244:TRP:CE2	2.56	0.41
1:D:88:HIS:HA	1:D:89:PRO:HD3	1.94	0.41
1:C:88:HIS:HE1	2:C:358:HOH:O	2.03	0.41
1:C:276:GLU:CD	1:C:276:GLU:H	2.28	0.41
1:D:88:HIS:CD2	1:D:90:ASN:H	2.39	0.40
1:B:216:LYS:HE2	1:B:292:GLU:O	2.20	0.40
1:B:152:ASN:HD22	1:B:152:ASN:C	2.29	0.40
1:D:228:ILE:O	1:D:249:ALA:HA	2.21	0.40
1:C:75:MET:HE3	1:C:236:MET:HA	2.03	0.40
1:A:183:PHE:HB3	1:A:214:TRP:CZ3	2.56	0.40
1:B:152:ASN:HD22	1:B:154:ALA:H	1.69	0.40
1:D:93:LYS:HG3	1:D:164:PHE:HD1	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/296 (95%)	269 (96%)	12 (4%)	0	100	100
1	B	287/296 (97%)	276 (96%)	10 (4%)	1 (0%)	36	17
1	C	291/296 (98%)	280 (96%)	11 (4%)	0	100	100
1	D	278/296 (94%)	268 (96%)	10 (4%)	0	100	100
All	All	1137/1184 (96%)	1093 (96%)	43 (4%)	1 (0%)	48	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/258 (96%)	247 (99%)	2 (1%)	73	54
1	B	253/258 (98%)	248 (98%)	5 (2%)	48	20
1	C	255/258 (99%)	252 (99%)	3 (1%)	63	38
1	D	243/258 (94%)	241 (99%)	2 (1%)	73	54
All	All	1000/1032 (97%)	988 (99%)	12 (1%)	63	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	PHE
1	A	236	MET
1	B	69	THR
1	B	152	ASN
1	B	169	ILE
1	B	212	ILE
1	B	236	MET
1	C	69	THR
1	C	236	MET
1	C	276	GLU
1	D	69	THR
1	D	236	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	27	ASN
1	A	77	HIS
1	A	136	GLN
1	A	279	HIS
1	B	12	GLN
1	B	46	GLN
1	B	53	ASN
1	B	77	HIS
1	B	88	HIS
1	B	111	HIS
1	B	152	ASN
1	B	181	HIS
1	B	279	HIS
1	C	15	GLN
1	C	77	HIS
1	C	88	HIS
1	C	178	GLN
1	C	189	GLN
1	C	279	HIS
1	D	12	GLN
1	D	15	GLN
1	D	26	ASN
1	D	42	GLN
1	D	77	HIS
1	D	88	HIS
1	D	111	HIS

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Mol	Chain	Res	Type
1	D	279	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	285/296 (96%)	0.57	19 (6%)	24	26	9, 16, 33, 55	0
1	B	291/296 (98%)	0.36	22 (7%)	20	21	8, 13, 29, 58	0
1	C	293/296 (98%)	0.22	13 (4%)	39	43	7, 13, 27, 46	0
1	D	282/296 (95%)	1.11	38 (13%)	7	7	11, 20, 37, 47	0
All	All	1151/1184 (97%)	0.56	92 (7%)	18	20	7, 15, 33, 58	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	ALA	9.2
1	A	182	LEU	9.1
1	D	4	LEU	7.9
1	A	183	PHE	7.8
1	B	175	THR	7.3
1	D	183	PHE	6.5
1	B	181	HIS	6.3
1	C	172	THR	6.3
1	D	13	PRO	6.2
1	A	214	TRP	6.2
1	D	214	TRP	5.8
1	B	296	MET	5.8
1	A	296	MET	5.5
1	C	4	LEU	5.3
1	A	295	LEU	4.9
1	A	4	LEU	4.6
1	D	11	LEU	4.4
1	D	7	LEU	4.3
1	A	2	ARG	4.3
1	A	171	SER	4.2
1	A	3	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	3	THR	3.9
1	D	12	GLN	3.9
1	B	214	TRP	3.9
1	A	184	THR	3.6
1	D	296	MET	3.6
1	D	15	GLN	3.6
1	A	5	LYS	3.5
1	C	44	ASP	3.4
1	B	4	LEU	3.4
1	B	171	SER	3.3
1	B	2	ARG	3.3
1	B	174	PRO	3.3
1	D	268	ASN	3.3
1	D	224	LYS	3.2
1	A	220	ARG	3.2
1	D	256	ILE	3.2
1	A	224	LYS	3.1
1	D	116	LYS	3.0
1	A	294	GLY	3.0
1	D	230	ARG	2.9
1	D	192	TYR	2.9
1	C	181	HIS	2.8
1	B	5	LYS	2.8
1	D	10	GLU	2.8
1	B	183	PHE	2.8
1	B	142	ASP	2.7
1	A	10	GLU	2.7
1	C	132	LYS	2.7
1	D	171	SER	2.7
1	A	268	ASN	2.6
1	A	155	GLU	2.6
1	D	267	PHE	2.6
1	C	5	LYS	2.6
1	D	93	LYS	2.6
1	D	197	GLU	2.6
1	D	295	LEU	2.5
1	D	266	LYS	2.5
1	D	142	ASP	2.5
1	B	172	THR	2.4
1	D	114	VAL	2.4
1	D	220	ARG	2.4
1	C	292	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	10	GLU	2.3
1	C	220	ARG	2.3
1	B	182	LEU	2.3
1	B	220	ARG	2.3
1	D	160	PHE	2.3
1	D	90	ASN	2.3
1	B	268	ASN	2.2
1	D	8	GLU	2.2
1	D	227	PRO	2.2
1	B	197	GLU	2.2
1	A	252	GLY	2.2
1	B	265	ARG	2.2
1	C	6	GLU	2.2
1	C	296	MET	2.2
1	B	36	ARG	2.1
1	A	186	GLU	2.1
1	C	161	LYS	2.1
1	D	5	LYS	2.1
1	D	6	GLU	2.1
1	D	264	VAL	2.1
1	C	173	ASP	2.1
1	D	144	PRO	2.1
1	D	184	THR	2.1
1	B	6	GLU	2.1
1	D	154	ALA	2.0
1	D	228	ILE	2.0
1	D	102	GLY	2.0
1	D	16	HIS	2.0
1	B	186	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.